

# Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 4-chloro-2-methoxyphenyl ester

<b>Inchi:</b>	InChI=1S/C17H15ClF8O5/c1-29-11-7-9(18)5-6-10(11)31-13(28)4-2-3-12(27)30-8-15(21,22)6
<b>InchiKey:</b>	BIPFNQRGCGDMAC-UHFFFAOYSA-N
<b>Formula:</b>	C17H15ClF8O5
<b>SMILES:</b>	COc1cc(Cl)ccc1OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
<b>Mol. weight [g/mol]:</b>	486.74

## Physical Properties

Property code	Value	Unit	Source
gf	-1951.76	kJ/mol	Joback Method
hf	-2418.59	kJ/mol	Joback Method
hfus	42.88	kJ/mol	Joback Method
hvap	71.33	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.138		Crippen Method
mcvol	273.780	ml/mol	McGowan Method
pc	1270.06	kPa	Joback Method
rinpol	2184.00		NIST Webbook
rinpol	2184.00		NIST Webbook
tb	821.46	K	Joback Method
tc	1010.62	K	Joback Method
tf	526.26	K	Joback Method
vc	1.099	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.89	J/molxK	821.46	Joback Method
cpg	834.05	J/molxK	852.99	Joback Method
cpg	844.32	J/molxK	884.51	Joback Method
cpg	853.75	J/molxK	916.04	Joback Method
cpg	862.38	J/molxK	947.57	Joback Method
cpg	870.25	J/molxK	979.10	Joback Method
cpg	877.43	J/molxK	1010.62	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U393901&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393901&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvp:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinp:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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